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IMPLEMENTING ADVANCED DATA ANALYSIS TECHNIQUES IN NEAR-REAL-TIME MATERIALS ACCOUNTING*

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ABSTRACT

Materials accounting for special nuclear material in fuel cycle facilities is implemented more efficiently by applying decision analysis methods, based on estimation and detection theory, to analyze process data for missing material. These methods are incorporated in the computer program DECANAL, which calculates sufficient statistics containing all accounting information, sets decision thresholds, and compares these statistics to the thresholds in testing the hypothesis H_0 of no missing material against the alternative H_1 that material is missing. DECANAL output provides alarm charts indicating the likelihood of missing material and plots of statistics that estimate materials loss. This program is a useful tool for aggregating and testing materials accounting data for timely detection of missing material.

I. INTRODUCTION

A. Purpose of Program

In developing conceptual designs for advanced materials accounting systems in nuclear fuel cycle facilities, the Safeguards Systems Group at the Los Alamos Scientific Laboratory has evolved a near-real-time materials accounting approach that combines on-line acquisition of process measurement data with advanced statistical methods in detecting existence of missing material and estimating the amount. A computer program (DECANAL) has been developed to implement these advanced statistical methods for accounting. DECANAL accepts measurement data, calculates materials balances and other indicators of missing material, and applies statistical tests to these indicators using a sequential statistical procedure that is adapted to the sequential nature of measurement data. Advantages inherent in such computerized data analysis are the processing of large amounts of data without error, rapid evaluation and reporting of statistical tests for timely detection of missing material, and the flexibility to isolate process areas

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selectively for analysis and spatially localized detection of missing material. The program DECANAL has been validated with data from numerous simulations of fuel cycle facilities. Most recently, it has been installed at the Allied-General Nuclear Services Plant (AGNS), where it has been used to evaluate in near-real time actual process data from cold runs.

During the development of DECANAL the philosophy has been to create a program that is general in its applicability to materials accounting problems, that is straightforward for the user to implement, and that has its output presented in a concise, easy-to-understand format. The program input format allows for any number of inventory and transfer measurements and correctly treats all correlations between measurements in calculating the materials balance and its variance, while requiring essentially the same kind of input data as for standard materials accounting practices. A preprocessing program (MASSAGE) removes any computational burden from the user by using the raw measurement data and information about the measurement variances to write an input data file for DECANAL. Output from DECANAL consists of indicators that allow the user to assess the likelihood of missing material and to estimate the amount of missing material.

B. Outline of Paper

Section II of this paper briefly describes the theory underlying the DECANAL program. The structure of the preprocessing program MASSAGE and the program DECANAL are discussed in section III. Section IV presents some of the practical problems encountered in implementing the decision analysis programs at the AGNS Facility, the solutions to these problems, and examples of the kinds of results to be expected when the programs become fully operational.

II. DECANAL METHODOLOGY

The estimation and detection methods embodied in DECANAL have been selected especially for their applicability to materials accounting problems. Because of the sequential nature of materials accounting data and the desirability of making a timely decision about missing material as the data become available, sequential estimation and detection procedures have been emphasized in DECANAL development. Also, because measurement data from a nuclear facility can show sizable run-to-run variability, methods that require comparison of current measurements to a reference or "normal" set of measurements for detection of process anomalies have been avoided. A detailed account of the theory underlying the program may be found in references 1-5.

DECANAL applies methods from decision analysis to detect the event of missing material, estimate the amount of missing material, and find the significance of that estimate. Detection of missing material is treated as a problem in statistical hypothesis testing where the hypothesis H_0 of no missing material is tested against the alternative hypothesis H_1 that some material is missing. The hypothesis H_1 incorporates a statement of the assumed materials loss mechanism, e.g., materials loss that is a uniform amount or a random amount in each period.

Because of the sequential time dependence of measurement data, the test of hypotheses is best implemented as a sequential test procedure. In an actual process, inventory and transfer measurements are collected in each balance period in addition to information about measurement errors. Denote the totality of this information for the k^{th} accounting period by $Z(k)$. The sequential test procedure in DECANAL requires the conditional probability densities of the information sequence $Z(1), Z(2), \ldots, Z(N)$ under each of the hypotheses. These densities are represented as

$$
\begin{aligned}
H_0&: \quad p_{z|H_0}(Z_1, \ldots, Z_N|H_0) \\
H_1&: \quad p_{z|H_1}(Z_1, \ldots, Z_N|H_1) \quad ,
\end{aligned}
\tag{1}
$$

where the conditional density $p_{z|H_0}$ reflects the assumed measurement behavior under normal operating conditions, and the conditional density $p_{z|H_1}$ reflects the behavior under some loss scenario, which requires assumptions about potential loss scenarios.

The test is applied in the form of a sequential probability ratio test (SPRT) that uses the decision rule[6]

$$
\text{If} \quad L(Z) = \frac{p_{z|H_1}(Z_1, \ldots, Z_N|H_1)}{p_{z|H_0}(Z_1, \ldots, Z_N|H_0)} \begin{cases} > T_1 & \text{accept } H_1 \\ < T_0 & \text{accept } H_0 \end{cases}
\tag{2}
$$

and for $T_0 \leq L(Z) \leq T_1$ defer a decision, observe the measurement data from the next accounting period, and apply the decision rule in Eq. (2). The ratio $L(Z)$ is called a likelihood ratio. The decision thresholds T_0 and T_1 are chosen so that the probabilities P_F of selecting H_1 when H_0 is true (false alarm) and P_M of selecting H_0 when H_1 is true (miss) do not exceed specified values. The SPRT has the advantage of reaching a decision with an expected number of observations that is less than that for a fixed-length test having the same P_M and P_F.

In some instances the statement of the hypotheses allows us to condense the data sequence $Z(1), Z(2), \ldots, Z(N)$ to a single number $S(N)$, called a sufficient statistic, that contains all of the information in the original sequence. DECANAL employs several sufficient statistics, each based on a different scenario for materials loss, and each sufficient statistic is the basis of a test for materials loss. Several of these tests are used to insure that all reasonable scenarios for materials loss are considered.

III. DECANAL STRUCTURE

A. MASSAGE Program

MASSAGE eases the user's computational burden by performing the routine calculations necessary for preparing a data input file for DECANAL. The MASSAGE program requires as input the basic process measurements such as concentrations, volumes, and flow rates, the random and systematic error variances associated with each measurement, and information describing which measurements are correlated. Such correlations could arise, for example, from measurements made with the same unrecalibrated instrument. This information is required because to calculate the variances of statistics such as the CUSUM correctly all correlations between measurements must be known.

The MASSAGE program combines the basic measurements into composite inventory and transfer measurements, as in the case of a tank where the program calculates the inventory as the product of a concentration and a volume measurement, and also calculates the random and systematic error variances of the product. Similarly, covariances between all inventory and transfer measurements are found. These inventory and transfer measurements, and their variances and covariances, constitute the input file for DECANAL.

B. DECANAL Program

DECANAL has three major functional components: the main program DECMN, the subroutine DECEST that contains the SPRTs in various forms, and the subroutine DECMSC that prints the results of the SPRTs. The main program reads the input data, prepared by MASSAGE, which includes inventory and transfer measurements, the variances of these measurements, and the covariances between measurements made at the same time and between measurements made sequentially in time. These data are used to calculate a materials balance and its variance for each time period. All of the measurement data and the materials balances are passed to DECEST for use in the SPRTs.

Because processing the large amounts of data from a process line can become prohibitive in computer storage and computation time when long sequences of measurement data are accumulated and manipulated, sufficient statistics that compress the original data sequence to a single number are useful. Some of the sufficient statistics used in DECANAL and the materials loss scenarios they represent are:

- CUSUM. Applicable to any materials loss scenario, this statistic is the cumulative sum of materials balances. The CUSUM statistic estimates total materials loss.

- Uniform Diversion. This statistic assumes a constant materials loss in each balance period and estimates the average materials loss per balance period with a Kalman filter.

- Smoothed Materials Balance. This statistic assumes a loss of material in some subset of contiguous materials balances. The statistic is calculated using forward and backward Kalman filters. The required accumulation of data delays a decision about missing material.

- Sequential Variance. Materials loss is assumed to be a random variable. Two Kalman filters are used to detect missing material through a change in the materials balance variance.

Because the exact form of a potential materials loss is uncertain, DECEST uses all of these sufficient statistics in a battery of SPRTs for missing material.

In DECEST each test is stored as a separate subroutine. The program user selects those tests to be used, and DECEST calls the test subroutines in their specified order. Because it is uncertain when a particular materials loss may begin and end, each test is applied to all contiguous subsequences of the total measurement data sequence. For each such subsequence the program applies the SPRT to detect a materials loss and calculates materials loss estimates.

After calculating the sufficient statistic for a data subsequence, DECEST calls the subroutine ALARM that compares the sufficient statistic to the decision thresholds for several false-alarm levels. When a decision threshold is exceeded, ALARM stores an indicator that shows the false-alarm level associated with the detection of missing material for that data subsequence. When all data subsequences have been processed for a particular test DECEST calls the next test, and the data analysis procedure is repeated.

At the completion of all tests requested by the user, the subroutine DECMSC is called to display the test results. Output from the subroutine DECMSC is intended to be useful in deciding if material is missing and in estimating the missing amount. The sufficient statistic associated with each test is plotted as a function of the balance periods. For the materials balance, CUSUM, and uniform diversion tests, these statistics represent the materials loss in a single period, the total loss up to the current period, and the average loss over all periods, respectively. The one-standard-deviation error in these estimates is also plotted at each point so that significant deviations of materials loss from the nominal value are easily detected. Results of applying the SPRT are plotted in the form of an alarm chart that summarizes the test result for each sequence of balance periods in which the sufficient statistic exceeded the decision threshold. This plot associates a symbol indicating the level of significance to each sequence that caused an alarm. Depending on the number of such alarms and their significance levels, a decision about materials loss is made.

IV. OPERATIONAL EXPERIENCE AT AGNS

Allied-General Nuclear Services at Barnwell, SC, is presently engaged in a series of cold runs at their reprocessing facility, which has the capability of processing uranium and plutonium in a copurification process as described in Fig. 1. During the course of these runs AGNS has provided the Los Alamos Scientific Laboratory's Safeguards Systems Group, Q-4, with the opportunity to acquire measurement data gathered by the AGNS computerized data acquisition system and to analyze the data in near-real time using the DECANAL program. Approximately 100 on-line measurement points can be interrogated by the AGNS system, with a new measurement acquired at each point at least every four minutes. For these cold runs, the DECANAL program is receiving data from 50 measurement points at about one-hour intervals.

Data analysis with the DECANAL program is being done on an AGNS-provided DEC PDP-11/34 time-sharing computer, which has a central memory of 264K words and the limitation that no program stored in central memory can exceed 32K words. A storage requirement of approximately 250K words for DECANAL has necessitated overlaying the program in 32-K segments so that it can be run on the AGNS machine.

For the purpose of applying near-real-time accounting to the process, we have formulated three unit process accounting areas (UPAAs): the full process, the columns and the concentrator, and the columns. Measurement data from each of the UPAAs are analyzed separately by the DECANAL program. By including the smaller UPAAs 60 to 80 kg U are controlled as compared with the approximately 425 kg U in the full process.

In implementing the DECANAL program with actual process data, we have become aware of certain difficulties that are inherent in near-real-time accounting; these are incorrect data from on-line measurement instruments and limitations on computer resources. Because of the hostile operational environment of most on-line instruments, malfunctions that cause incorrect measurements must be expected. Such erroneous measurements entered into the data base can produce false indications of excess or missing material, so in DECANAL data errors are removed through a system of error checks that include: comparing the on-line measurement to a laboratory analysis when available; comparing measurements made in two different ways, e.g., the total amount of material transferred out of a tank could be calculated from a concentration and volume measurement in the tank, and a concentration and flow measurement in the output transfer stream; or by determining if the measurement is within reasonable bounds established by historical measurement data.

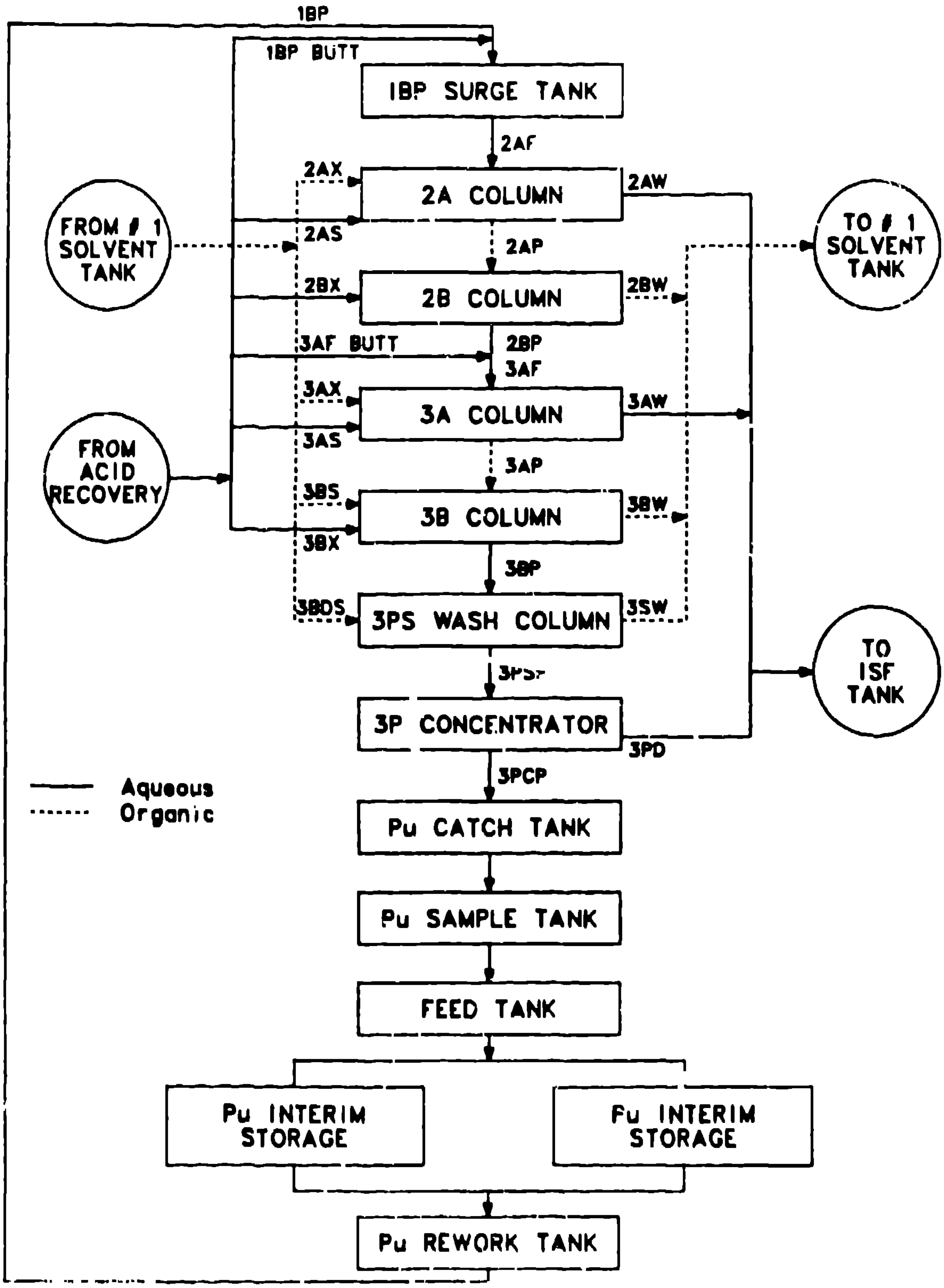
Because of the large amounts of data that are potentially available from on-line instruments and laboratory analyses in a fully instrumented nuclear facility, computer storage and computational time can become limited, especially over long time intervals. A method for avoiding such computer resource limitations is data compression; for example, if there are several inventory measurements that are uncorrelated with all other measurements, these may be summed into a single measurement and treated as a single piece of information throughout the calculations. Data combined in this way conserve computer storage and reduce computational time.

While the first results from the AGNS work are not yet available, it is possible to describe the expected results with DECANAL output from process simulations. For this purpose, the entire process is chosen as the UPAA. Process simulations were used to generate two sets of measurement data; one in which the process operates normally and another in which a uniform amount of material is diverted during each balance period. Results of applying the uniform diversion test to the two data sets are shown in Fig. 2 as plots of the average materials loss per balance period and alarm charts. For normal process operation the loss estimator converges to the true value of zero, while for the uniform diversion case the estimator approaches the true value of 0.3 kg missing per balance period. Note that the alarm chart for the diversion scenario strongly indicates missing material through the large number of significant alarms. The formulation and interpretation of these alarm charts have been described in previous papers.

V. SUMMARY

DECANAL provides a useful tool for performing advanced data analysis in a near-real-time materials accounting framework. Although this computer program requires very little more input data than is necessary for conventional accounting purposes, it provides the flexibility to analyze process UPAAs selectively in near-real time so that any missing material is spatially localized and the estimate of missing material is timely.

Figure 1. U/Pu Copurification Process.



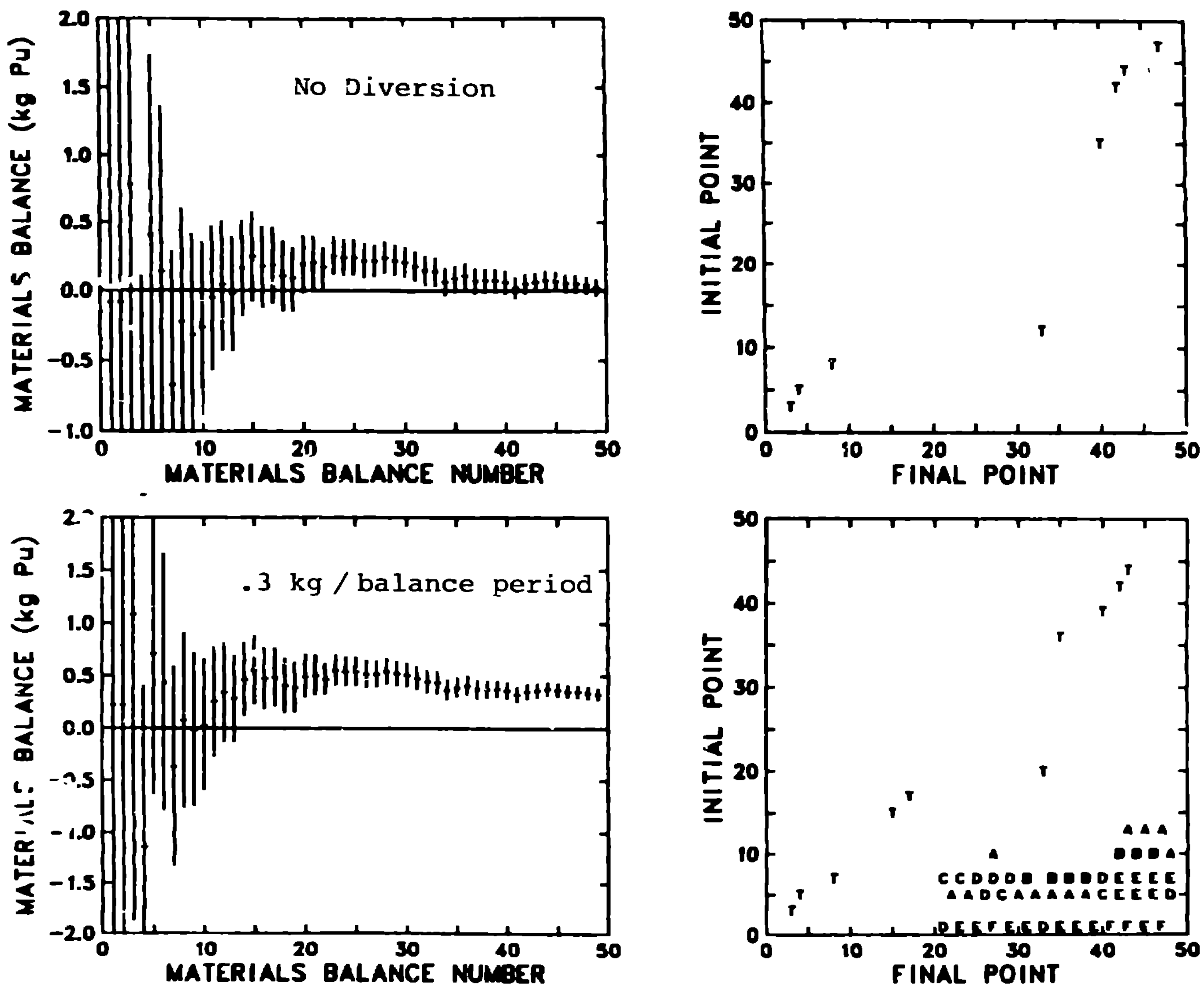


Fig. 2. Uniform Diversion Test Results

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